



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:43 PM GMT

PDB ID : 1QAS
Title : 1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODI-
ESTERASE DELTA 1
Authors : Grobler, J.A.; Hurley, J.H.
Deposited on : 1996-08-02
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

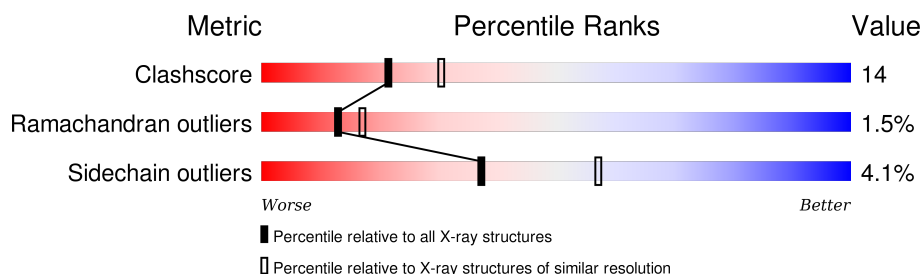
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	622	
1	B	622	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8235 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOSPHOLIPASE C DELTA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3990	2522	696	750	22			
1	B	504	Total	C	N	O	S	0	0	0
			3979	2517	696	744	22			

- Molecule 2 is water.

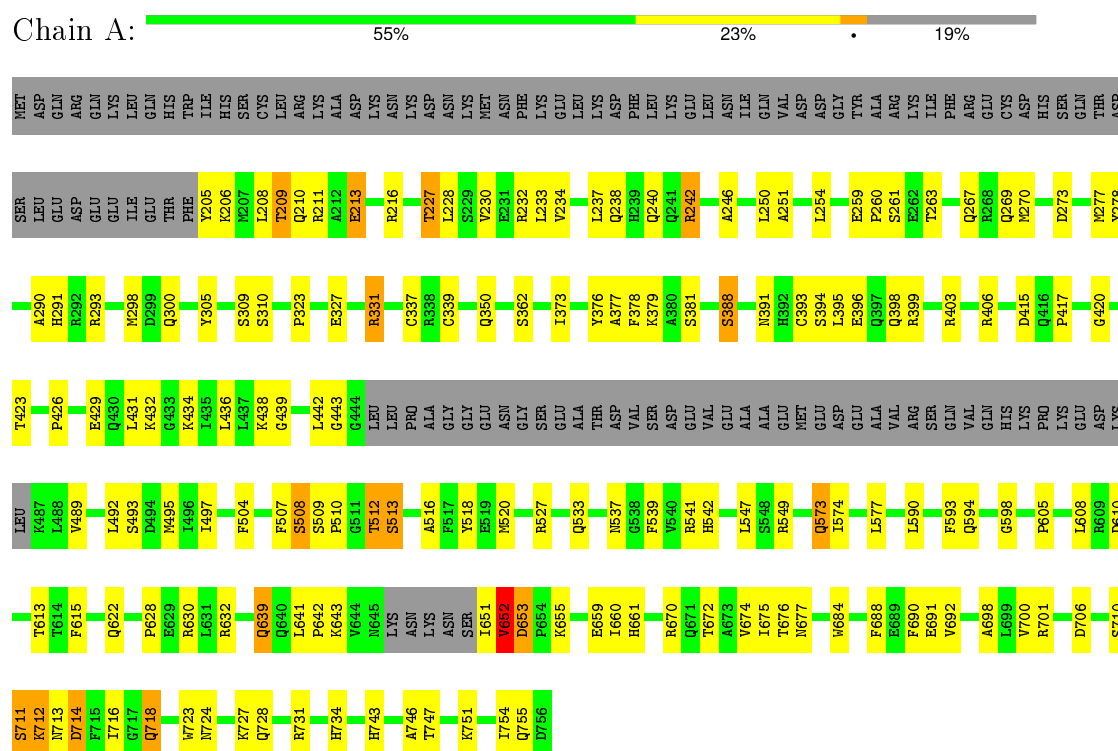
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		
2	B	134	Total	O	0	0
			134	134		

3 Residue-property plots

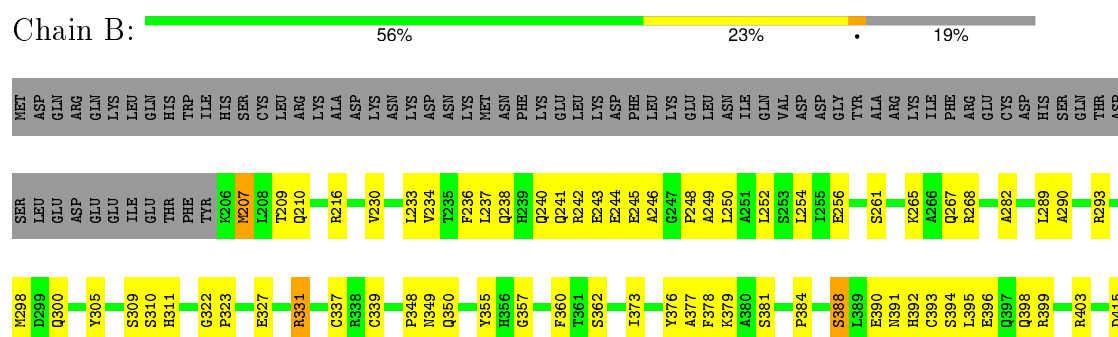
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: PHOSPHOLIPASE C DELTA-1



• Molecule 1: PHOSPHOLIPASE C DELTA-1



D714	T423	L492	P426	E429	Q430	L431	K432	Q433	K434	F435	L436	L437	K438	Q439	G443	G444	L445	LEU	PRO	ALA	GLY	GLY	GLU	ASN	GLY	SER	GLU	ALA	THR	ASP	VAL	SER	ASP	GLU	VAL	GLU	ALA	ALA	ALA	GLU	MET	GLU	ASP	GLU	ALA	VAL	ARG	SER	GLN	VAL	GLN	HIS	LYS	PRO	LYS	GLU	ASP	K495
S617	M495	I496	I497	K500	F504	F507	S508	S509	P510	GLY	THR	SER	Q514	Q515	A516	F517	Y518	E519	M520	E525	S526	R527	N537	G538	F539	L547	S548	R549	P552	A553	Q573	I574	L590	F593	Q594	G598	P605	L608	R609	D610	T613	T614	F615															
M616	Q622	P628	E629	R630	I636	Q639	Q640	L641	P642	K643	N644	N645	LYS	ASN	LYS	ASN	SER	T651	V652	D653	P654	E659	T660	R661	G662	R670	Q671	T672	L675	T676	R677	N684	F688	E689	E690	E691	V692	L698	L699	V700	R701	D706	S710	S711	K712	N713												
Q718	V723	K727	Q728	Q729	Y730	R731	H734	H743	A746	I754	Q755	D756																																														

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.10Å 75.40Å 86.90Å 66.90° 85.40° 89.80°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8235	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/4083	0.79	5/5531 (0.1%)
1	B	0.52	0/4070	0.78	5/5511 (0.1%)
All	All	0.51	0/8153	0.78	10/11042 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	331	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	A	331	ARG	NE-CZ-NH1	14.68	127.64	120.30
1	B	331	ARG	NE-CZ-NH2	-13.39	113.60	120.30
1	B	331	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	331	ARG	CD-NE-CZ	7.38	133.93	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3990	0	3906	118	0
1	B	3979	0	3903	109	0
2	A	132	0	0	5	0
2	B	134	0	0	7	0
All	All	8235	0	7809	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 222 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.47	0.95
1:A:228:LEU:HB2	1:A:270:MET:HB3	1.47	0.94
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.60	0.82
1:A:399:ARG:O	1:A:403:ARG:HG2	1.79	0.82
1:A:573:GLN:H	1:A:573:GLN:HE21	1.31	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/622 (80%)	458 (92%)	31 (6%)	10 (2%)	9	11
1	B	496/622 (80%)	462 (93%)	29 (6%)	5 (1%)	19	28
All	All	995/1244 (80%)	920 (92%)	60 (6%)	15 (2%)	13	17

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	513	SER
1	A	711	SER
1	B	711	SER
1	A	508	SER
1	A	512	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	437/544 (80%)	418 (96%)	19 (4%)	35	55
1	B	435/544 (80%)	418 (96%)	17 (4%)	39	59
All	All	872/1088 (80%)	836 (96%)	36 (4%)	37	57

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	691	GLU
1	B	242	ARG
1	B	691	GLU
1	A	718	GLN
1	B	254	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	639	GLN
1	A	734	HIS
1	B	718	GLN
1	A	718	GLN
1	A	728	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.